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S6	9	RD (unique items)
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7/AB/1 (Item 1 from file: 155)
 DIALOG(R) File 155:MEDLINE(R)
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10261806 PMID: 7525561

Identification of the regulatory domain of the mammalian multifunctional protein **CAD** by the construction of an Escherichia coli hamster hybrid carbamyl-phosphate synthetase.

Liu X; Guy H I; Evans D R
 Department of Biochemistry, Wayne State University School of Medicine, Detroit, Michigan 48201.

Journal of biological chemistry (UNITED STATES) Nov 4 1994, 269 (44) p27747-55, ISSN 0021-9258 Journal Code: 2985121R

Contract/Grant No.: GM 47399; GM; NIGMS

Document type: Journal Article

Languages: ENGLISH

Main Citation Owner: NLM

Record type: Completed

Carbamyl-phosphate synthetases from different organisms have similar catalytic mechanisms and amino acid sequences, but their structural organization, sub-unit structure, and mode of regulation can be very different. Escherichia coli carbamyl-phosphate **synthetase** (CPSase), a monofunctional **protein** consisting of amido-transferase and **synthetase** subunits, is allosterically inhibited by UMP and activated by NH3, IMP, and ornithine. In contrast, mammalian CPSase II, part of the

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ACCESSION NUMBER: 2001:303055 HCAPLUS

DOCUMENT NUMBER: 135:101926

TITLE: Design of inhibitors of Ras-Raf interaction using a
computational combinatorial algorithmAUTHOR(S): Zeng, Jun; Nheu, Thao; Zorzet, Anna; Catimel, Bruno;
Nice, Ed; Maruta, Hiroshi; Burgess, Antony W.;
Treutlein, Herbert R.CORPORATE SOURCE: Ludwig Institute for Cancer Research, Royal Melbourne
Hospital, Parkville, 3050, Australia

SOURCE: Protein Engineering (2001), 14(1), 39-45

CODEN: PRENE9; ISSN: 0269-2139

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Drugs that inhibit important **protein-protein**
 interactions are hard to find either by screening or rational design, at
 least so far. Most drugs on the market that target **proteins**
 today are therefore aimed at well-defined binding pockets in
proteins. While **computer-aided design**
 is widely used to facilitate the drug discovery process for binding
 pockets, its application to the design of inhibitors that target the
protein surface initially seems to be limited because of the
 increased complexity of the task. Previously, we had started to develop a
 computational combinatorial design approach based on the well-known
 "multiple copy simultaneous search" (MCSS) procedure to tackle this
 problem. In order to identify sequence patterns of potential inhibitor
peptides, a three-step procedure is employed: first, using MCSS,
 the locations of specific functional groups on the **protein**
 surface are identified; second, after constructing the **peptide**
 main chain based on the location of favorite locations of
 N-methylacetamide groups, functional groups corresponding to amino acid
 side chains are selected and connected to the main chain C α atoms;
 finally, the **peptides** generated in the second step are aligned
 and probabilities of amino acids at each position are calculated from the
 alignment scheme. Sequence patterns of potential inhibitors are determined
 based on the propensities of amino acids at each C α position. Here